

Diethyl ether

60-29-7 | DTXSID3021720

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 39.0 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 8.36e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diethyl ether</div> <div>Measured: 34.6</div> <div>Predicted: 39.0</div>	<div>Image not found</div> <div>Propane, 1-methoxy-</div> <div>Measured: 39.1</div> <div>Predicted: 39.0</div>	<div>Image not found</div> <div>Ether, isopropyl methyl</div> <div>Measured: 30.7</div> <div>Predicted: 35.1</div>
<div>Image not found</div> <div>2-Chlorobutane</div> <div>Measured: 68.0</div> <div>Predicted: 63.8</div>	<div>Image not found</div> <div>t-Butylchloride</div> <div>Measured: 50.5</div> <div>Predicted: 58.0</div>	<div>Image not found</div> <div>(2H9)-tert-Butyl chloride</div> <div>Measured: 50.5</div> <div>Predicted: 58.0</div>